The influence of single magnetic impurities on the conductance of quantum microconstrictions.

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Abstract

The nonlinear ballistic conductance of three-dimensional quantum microconstrictions, which contain magnetic impurities, is investigated. The nonlinear part of the conductance, which is due to the interaction of electrons with magnetic impurities is obtained. The analytical results have been analyzed numerically. It is shown that intensity of the Kondo anomaly in the conductance as the function of the applied voltage depends on the diameter of the constriction and the positions of impurities.

The impurity-electron interaction in Kondo systems can be effectively studied by using the point contacts (PC). In first measurements of the differential PC resistance $R(V)$ in metals with magnetic impurities the zero-bias Kondo anomaly had been observed [1–3]. These experiments were explained by quasiclassical theory of Kondo effect in PC's [4]. It was shown that in second-order Born approximation the magnetic impurity contribution to the PC resistance includes the logarithmic dependence $R(V) \sim \ln(V)$ for $eV \gg T_K$ and

the saturation for $eV \ll T_K$ (T_K is the Kondo temperature, V is the voltage applied to the PC). In accordance to the theory [4], the nonlinear correction to the ballistic PC resistance is proportional to the contact diameter. But in the experiments [1–3] the size dependence of the PC current was not investigated due to the limited range of contact diameters, which were accessible.

The development of the technique of mechanically controllable break junctions (MCBJ) has made it possible to create the stable PC's, with the diameter adjustable over broad range, down to a single atom [5,6]. In the MCBJ experiments [7,8] authors had studied the resistance of ultrasmall contacts with magnetic impurities as function of the PC diameter d. In the contrast to the prediction of the quasiclassical theory [4] Yanson at el. [7,8] observed that Kondo scattering contribution to the contact resistance is nearly independent from the contact diameter d for small d. Such behavior authors [7,8] had explained by the increasing of Kondo impurity scattering cross-section with decreasing of contact size.

In theoretical works [9] it was shown that in very small contacts the discreteness of impurity positions must be taken into account, and experiments [7,8] may be explained by the "classical" mesoscopic effect of the dependence of the point contact conductance on the spatial distribution of impurities. This effect is essential in the "short" contacts and in the quasiclassical approximation it disappears with the increasing of the contact length. Zarand and Udvardi [10] had considered the contact in the in the form of a long channel and suggested that the Kondo temperature T_K is changed due to the strong the local density of states fluctuations generated by the reflections of conduction electrons at the surface of the contact. As a result of that, the effective cross section of electrons has the maximum, if the position of the impurity inside the contact corresponds to the maximum in the local electron density of states. But the mesoscopic effect of the spatial distribution of impurities in quantum contacts was not analyzed in the paper [10].

In ultrasmall contacts the quantum phenomena, which are known as quantum size effect, occur. The effect of the $2e^2/h$ conductance quantization has been observed in experiments on contacts in the two-dimensional electron gas [11,12] and in the ultrasmall three-dimensional

constrictions, which is created by using the scanning tunnel microscopy [13,14] and mechanically controllable break junctions [15]. The defects produce the backscattering of electrons, and thus break the quantization of the conductance. From the other hand, the impurities situated inside the quantum microconstriction produce the nonlinear dependence of the conductance on the applied voltage [18]. This dependence is the result of the interference of electron waves reflected by these defects [16,17].

In this paper we present the theoretical solution of this problem for the conductance of a quantum microconstriction in the form of the long ballistic channel , which contains single magnetic impurities. The study is made of the first and second order corrections to the conductance of the ballistic microconstriction in the Born approximation. The effect of impurity positions is taken into account. Within the framework of the model of the long channel the quantum formula for the conductance G is obtained. By using the model of the cylindrical microconstriction, the nonlinear conductance as a function of voltage V and the width of constriction d is analyzed numerically for different positions of a single impurity.

Let us consider the quantum microconstriction in the form of a long and perfectly clean channel with smooth boundaries and a diameter d comparable with the Fermi wave length $\lambda_F = h/\sqrt{2m\varepsilon_F}$, where ε_F is the Fermi energy. We assume that this channel is smoothly (over Fermi length scale) connected with a bulk metal banks. As it was shown [20,21], in such constriction in the zeroth approximation on the adiabatic parameter $|\nabla d| \ll 1$ accurate quantization can be obtained. The corrections to the tunneling and reflection coefficients of electrons due to deviation from the adiabatic constriction are exponentially small, except near the points where the modes are switched on and off [22].

When a voltage V is applied to the constriction, a net current start to flow. In the limit $V \to 0$, the ballistic conductance of the quantum microconstriction is given by the formula

$$G = \frac{dJ}{dV} = G_0 \sum_{\beta} f_F\left(\varepsilon_\beta\right), \tag{1}$$

where f_F is the Fermi function, ε_β is the minimal energy of the transverse electron mode, β is the full set of transverse discrete quantum numbers. The ballistic quantum PC displays the

specific nonlinear properties, such as the conductance jumps e^2/h. For the two dimensional PC these effects was considered in the papers [23,24]. The aim of this study is to analyze the zero bias Kondo minimum in the PC conductance. We assume that the bias eV is much smaller not only the Fermi energy ε_F, but also the distances between the energies ε_β of quantum modes. In this case the effect of the influence of the applied bias to the transmission is negligibly small.

Impurities and defects scatter the electrons that leads to the decreasing of the transmission probability. In accordance with the standard procedure [25,26] the decreasing of the electrical current ΔI due to the electron-impurity interaction connects with the velocity of the energy E dissipation by the relation:

$$\Delta IV = \frac{dE}{dt} = \frac{d\left\langle H_1 \right\rangle}{dt}; \tag{2}$$

The Hamiltonian of the electrons H contains the following terms:.

$$H = H_0 + H_1 + H_{int}, \tag{3}$$

where

$$H_0 = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \tag{4}$$

is Hamiltonian of free electrons,

$$H_1 = \frac{eV}{2} \sum_{k,\sigma} sign(v_z) c^\dagger_{k\sigma} c_{k\sigma} \tag{5}$$

describes the interaction of electrons with electric field. The Hamiltonian of the interaction of electrons with magnetic impurities H_{int} can be written as

$$H_{int} = \sum_{j,k,k'} \mathbf{J}_{j,k,k'} \left[S_z \left(c^\dagger_{k'\uparrow} c_{k\uparrow} - c^\dagger_{k'\downarrow} c_{k\downarrow} \right) + S^- c^\dagger_{k'\uparrow} c_{k\downarrow} + + S^+ c^\dagger_{k'\downarrow} c_{k\uparrow} \right]. \tag{6}$$

Here the operator $c_{k\sigma}^{+}$ $(c_{k\sigma})$ creates (annihilates) a conduction electron with spin σ, wave function φ_k, and energy ε_k; $\mathbf{S}$ denotes the spin of impurity; v_z is the electron velocity along the channel; $\mathbf{J}_{j,k,k'}$ is the matrix element of the exchange interaction of electron with impurity in the point $\mathbf{r}_j$; $k\sigma$ is the full set of quantum numbers;

$$\mathbf{J}_{j,k,k'} = \int d\mathbf{r}\ J(\mathbf{r},\mathbf{r}_j)\varphi_k(\mathbf{r})\varphi_{k'}^{*}(\mathbf{r}). \tag{7}$$

The electron wave functions and eigenvalues in the long channel in the adiabatic approximation are

$$\varphi_k(\mathbf{r}) = \psi_\beta(\mathbf{R}) \exp\left(\frac{i}{\hbar} p_z z\right); \tag{8}$$

$$\varepsilon_k = \varepsilon_\beta + \frac{p_z^2}{2m_e}; \tag{9}$$

where $k = (\beta, p_z)$, β is the set of discrete transverse quantum numbers; p_z is the momentum of an electron along the contact axis; m_e is an electron mass; $\mathbf{r} = (\mathbf{R}, z)$, $\mathbf{R}$ is a coordinate in the plain, perpendicular to the z axis.

Differentiating $\langle H_1 \rangle$ over the time t we obtain the equation for the changing ΔI of the current as a result of the interaction of electrons with magnetic impurities:

$$V\Delta I = \frac{1}{i\hbar} \left\langle \left[H_1(t), H_{int}(t) \right] \right\rangle, \tag{10}$$

where

$$\langle ... \rangle = Tr\left(\rho(t) ...\right). \tag{11}$$

All operators are in the representation of interaction.

The statistical operator $\rho(t)$ satisfies to equation

$$i\hbar \frac{\partial \rho}{\partial t} = \left[H_{int}(t), \rho(t) \right], \tag{12}$$

which can be solved using the perturbation theory:

$$\rho(t) = \rho_0 + \frac{1}{i\hbar}\int\limits_{-\infty}^{t} dt' \left[H_{int}(t'), \rho_0\right] + \frac{1}{(i\hbar)^2}\int\limits_{-\infty}^{t} dt' \int\limits_{-\infty}^{t'} dt'' \left[H_{int}(t'), \left[H_{int}(t''), \rho_0\right]\right]\cdots \tag{13}$$

By means of Eq.(13) the changing in the electric current due to magnetic impurities can be determined

$$\Delta I = I_1 + I_2 + ... = \tag{14}$$

$$-\frac{1}{\hbar^2 V}\int\limits_{-\infty}^{t} dt' Tr\left(\rho_0\left[\left[H_1, H_{int}(t)\right], H_{int}(t')\right]\right) -$$

$$-\frac{1}{i\hbar^3 V}\int\limits_{-\infty}^{t'} dt'' \int\limits_{-\infty}^{t} dt' Tr\left(\rho_0\left[\left[\left[H_1, H_{int}(t)\right], H_{int}(t')\right], H_{int}(t'')\right]\right) + ...$$

After the simple, but cumbersome calculations we find the first and second order corrections to the PC current

$$I_1 = -\frac{e\pi}{\hbar} s(s+1) \sum_{n,m}\sum_{i,j} (sign\ v_{z_m} - sign\ v_{z_n})(f_m - f_n)\ \ \delta(\varepsilon_n - \varepsilon_m)\ \mathbf{J}_{j,n,m}\, \mathbf{J}_{i,m,n}; \tag{15}$$

$$I_2 = \frac{\pi e}{\hbar} s(s+1) \sum_{n,m,k}\sum_{i,j,l} (sign\ v_{z_k} - sign\ v_{z_n}) \tag{16}$$

$$[\delta(\varepsilon_n - \varepsilon_k)\,\mathrm{Pr}\ \frac{1}{\varepsilon_m - \varepsilon_k} + \delta(\varepsilon_m - \varepsilon_k)\,\mathrm{Pr}\ \frac{1}{\varepsilon_n - \varepsilon_k}]$$

$$[\mathbf{J}_{j,n,k}\mathbf{J}_{i,m,n}\mathbf{J}_{l,k,m} + \mathbf{J}_{j,k,n}\mathbf{J}_{i,n,m}\mathbf{J}_{l,m,k}]$$

$$[2f_n(f_k - f_m) + (f_m - f_k)],$$

where $f_n = f_F\left(\varepsilon_n + \frac{eV}{2} sign v_z\right)$. The first addition I_1 to the PC current describes the small spin-depended correction (of the order $(J/\varepsilon_F)^2$) to the changing of the current due to the usual scattering. The second addition I_2 is also small too, but contains the Kondo

logarithmic dependence on the voltage, and it is most important for the analysis of the nonlinear conductance of constrictions with magnetic impurities.

The expressions (15) and (16) can be further simplified in the case of $\delta-$potential of impurities

$$J(\mathbf{r}) = J\delta(\mathbf{r}) \tag{17}$$

In this case the addition I_2 to the ballistic current has the form:

$$\begin{gathered} I_2 = \frac{2J^3\pi e}{\hbar} s(s+1) \sum_{n,m,k} \sum_{i,j,l} (sign\ v_{z_k} - sign\ v_{z_n}) \\ [\delta(\varepsilon_n - \varepsilon_k) \operatorname{Pr} \frac{1}{\varepsilon_m - \varepsilon_k} + \delta(\varepsilon_m - \varepsilon_k) \operatorname{Pr} \frac{1}{\varepsilon_n - \varepsilon_k}] \\ \operatorname{Re}[\varphi_k^*(\mathbf{r}_j)\varphi_n^*(\mathbf{r}_i)\varphi_m^*(\mathbf{r}_l)\varphi_k(\mathbf{r}_l)\varphi_m(\mathbf{r}_i)\varphi_n(\mathbf{r}_j)] \\ [2f_n(f_k - f_m) + (f_m - f_k)], \end{gathered} \tag{18}$$

As it follows from the Eqs.(16), (18), the current I_2 depends from the positions of impurities. Two effects influence by value I_2 : the effect of quantum interference of scattered electron waves, which depends from the distances between impurities, and effect of the electron density of states in the points, where the impurities are situated. The nonlinear part of the conductance can be easy obtained after differentiation the Eq.18 over the voltage $G_2 = dI_2/dV$. In the case of a single impurity and at zero temperature $T = 0$ this equation can be analytically integrated over momentum p_z and the conductance G_2 takes the following form:

$$\begin{gathered} G_2 = -\frac{\pi e^2 m_e^3}{\hbar^4} J^3 s(s+1) \sum_{\alpha,\beta,\gamma} \sum_{\varkappa=\pm} |\psi_\alpha(\mathbf{R})|^2 |\psi_\beta(\mathbf{R})|^2 |\psi_\beta(\mathbf{R})|^2 \left[p_\alpha^{(\varkappa)} p_\beta^{(\varkappa)} p_\gamma^{(\varkappa)}\right]^{-1} \cdot \\ \left[\ln\left|\frac{p_\gamma^{(\varkappa)} - p_\gamma^{(-\varkappa)}}{p_\gamma^{(\varkappa)} + p_\gamma^{(-\varkappa)}} \left(\frac{p_\alpha^{(\varkappa)}}{p_\gamma^{(\varkappa)}}\right)\right| + (1-\delta_{\alpha\beta}) \ln\left|\frac{p_\alpha^{(\varkappa)} p_\beta^{(-\varkappa)} - p_\alpha^{(-\varkappa)} p_\beta^{(\varkappa)}}{p_\alpha^{(\varkappa)} p_\beta^{(-\varkappa)} + p_\alpha^{(-\varkappa)} p_\beta^{(\varkappa)}}\right| + \right. \\ \left. \delta_{\alpha\beta} \ln\left|\frac{\left(p_\alpha^{(\varkappa)}\right)^2 - \left(p_\alpha^{(-\varkappa)}\right)^2}{\left(p_\alpha^{(-\varkappa)}\right)^2}\right|\right]; \end{gathered} \tag{19}$$

where

$$p_{\alpha}^{(\pm)} = \sqrt{2m_e \left(\varepsilon_F \pm \frac{eV}{2} - \varepsilon_\alpha \right)}, \tag{20}$$

and the transverse parts of the wavefunction $\psi_\alpha(\mathbf{R})$ and the electron energy ε_α are defined by Eqs. (8), (9).

Carrying out the numerical calculations we use the free electron model of a point contact consisting of two infinite half-spaces connected by a long ballistic cylinder of a radius R and a length L (Fig.1). In a limit $L \rightarrow \infty$ the electron wave functions $\varphi_k(\mathbf{r})$ and eigenstates ε_k can be written as

$$\varphi_k(\mathbf{r}) = \frac{1}{\sqrt{\Omega} J_{m+1}(\gamma_{mn})} J_m\left(\gamma_{mn} \frac{\rho}{R}\right) \exp\left(im\varphi + \frac{i}{\hbar} p_z z\right); \tag{21}$$

$$\varepsilon_k = \varepsilon_{mn} + \frac{p_z^2}{2m_e}; \quad \varepsilon_{mn} = \frac{\hbar^2}{2m_e R^2} \gamma_{mn}^2 \tag{22}$$

and cylindrical coordinates $\mathbf{r} = (\rho, \varphi, z)$ with the axis z along the channel axis have been used. Here $k = (n, m, p_z)$ are the quantum numbers, $\Omega = \pi R^2 L$ is the volume of the channel, γ_{mn} are the n-th zero of the Bessel function J_m. Because the degeneration of the electron energy on azimuthal quantum number m (as a result of the symmetry of the model), quantum modes with $\pm m$ give the same contribution to the conductance. In this model the ballistic conductance (1) has not only steps G_0, but also steps $2G_0$ [21,27].

In Fig.2 the dependence of the nonlinear conductance on the applied bias is shown for the different positions of a single magnetic impurity inside the channel. The results obtained confirm that the nonlinear effect is strongly depend on the position of impurity. If the impurity is situated near the surface of the constriction $\mathbf{r} = \mathbf{R}$, where the square module of the electron wave function is small, its influence to the conductivity is negligible. This conclusion is confirmed by the calculations of the dependence G_2 on the position of the impurity for different number of quantum modes (Fig.3). Results indicate that the

mesoscopic effect of the impurity position is more essential for ultrasmall contacts, which contain only few conducting modes, and G_2 has a maximum. The similar results is obtained for the dependence of G_2 on the radius R of the constriction (Figs.4,5). In the single-mode constriction (Fig.4) the conductance G_2 displays much more stronger dependence on R, than in the contact with five conducting modes (Fig.5).

Thus, we have shown that in the long quantum microconstrictions the spatial distribution of magnetic impurities influences to the nonlinear dependence of the conductance on the applied voltage. This mesoscopic effect is due to the strong dependence the amplitude of an electron scattering on the positions of impurities. As a result of the reflection from the boundaries of the constriction the electron wave functions, which correspond to the finite electron motion in the transverse to the contact axis direction, are the standing waves. If the impurity is situated near the point, in which the electron wave function is equal to zero (near the surface of the constriction or, for quantum modes with numbers $n > 1$, in some points inside), its scattering of electrons is small. The fact the amplitude of the Kondo minimum of the conductance of the quantum contact display the mesoscopic effect of the dependence on the positions of single impurities. This effect is most important in the case, when only few quantum modes are responsible on the conductivity of the constriction.

Figure captions.

Fig. 1. Schematic representation of a ballistic microconstriction in the form of a long channel, adiabatically connected to large metallic reservoirs. Magnetic impurities inside the constriction are shown.

Fig. 2. The voltage dependence of the nonlinear part of conductance G_2 (19) from the distance of the impurity from the contact axis ($2\pi R = 5.2\lambda_F$; $T = 0$; 1 - $2\pi\rho = 1.5\lambda_F$; 2 -$2\pi\rho = 2.5\lambda_F$; 3 -$2\pi\rho = 3.0\lambda_F$; 4 - $2\pi\rho = 3.5\lambda_F$).

Fig. 3. The dependence of G_2 (19) on the position of the impurity for the different quantum modes in the constriction ($V = 0.02\varepsilon_F$; $T = 0$; 1 - one mode ($2\pi R = 3\lambda_F$); 2 - three modes($2\pi R = 4\lambda_F$); 3 - five modes ($2\pi R = 5.3\lambda_F$); 4 - six modes ($2\pi R = 6\lambda_F$)).

Fig. 4. The dependence of G_2 (19) on the radius of the constriction for the single mode channel and different positions of the impurity ($V = 0.02\varepsilon_F; T = 0$;1 - $2\pi\rho = 0.5\lambda_F$; 2 -$2\pi\rho = 1.0\lambda_F$; 3 -$2\pi\rho = 1.5\lambda_F$; 4 - $2\pi\rho = 2.0\lambda_F$)

Fig. 5. The dependence of G_2 on the radius for the microconstriction with five quantum modes and different positions of the impurity ($V = 0.02\varepsilon_F; T = 0$;1 - $2\pi\rho = 0.5\lambda_F$; 2 -$2\pi\rho = 1.5\lambda_F$; 3 -$2\pi\rho = 2.5\lambda_F$; 4 - $2\pi\rho = 4.5\lambda_F$)

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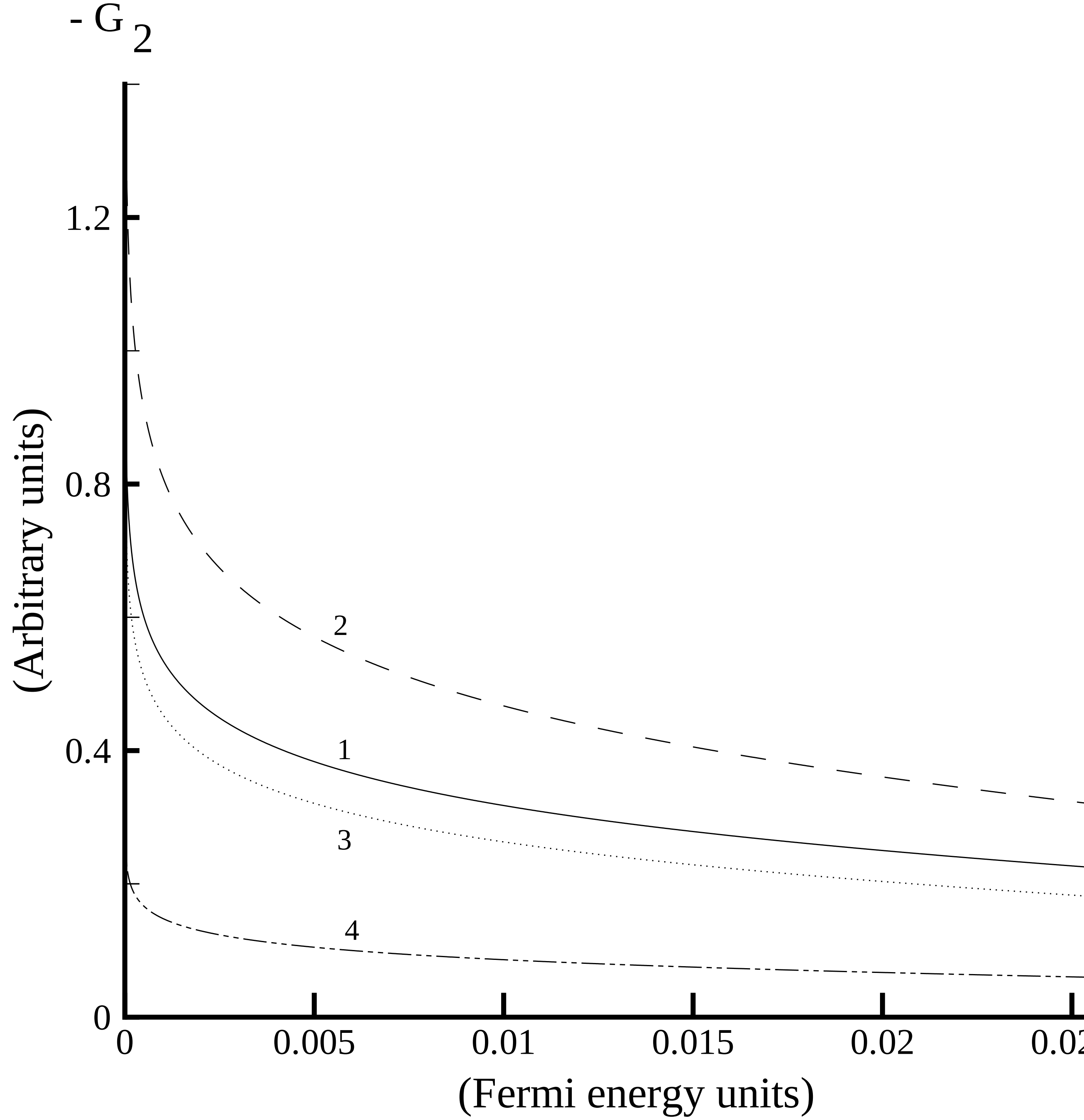
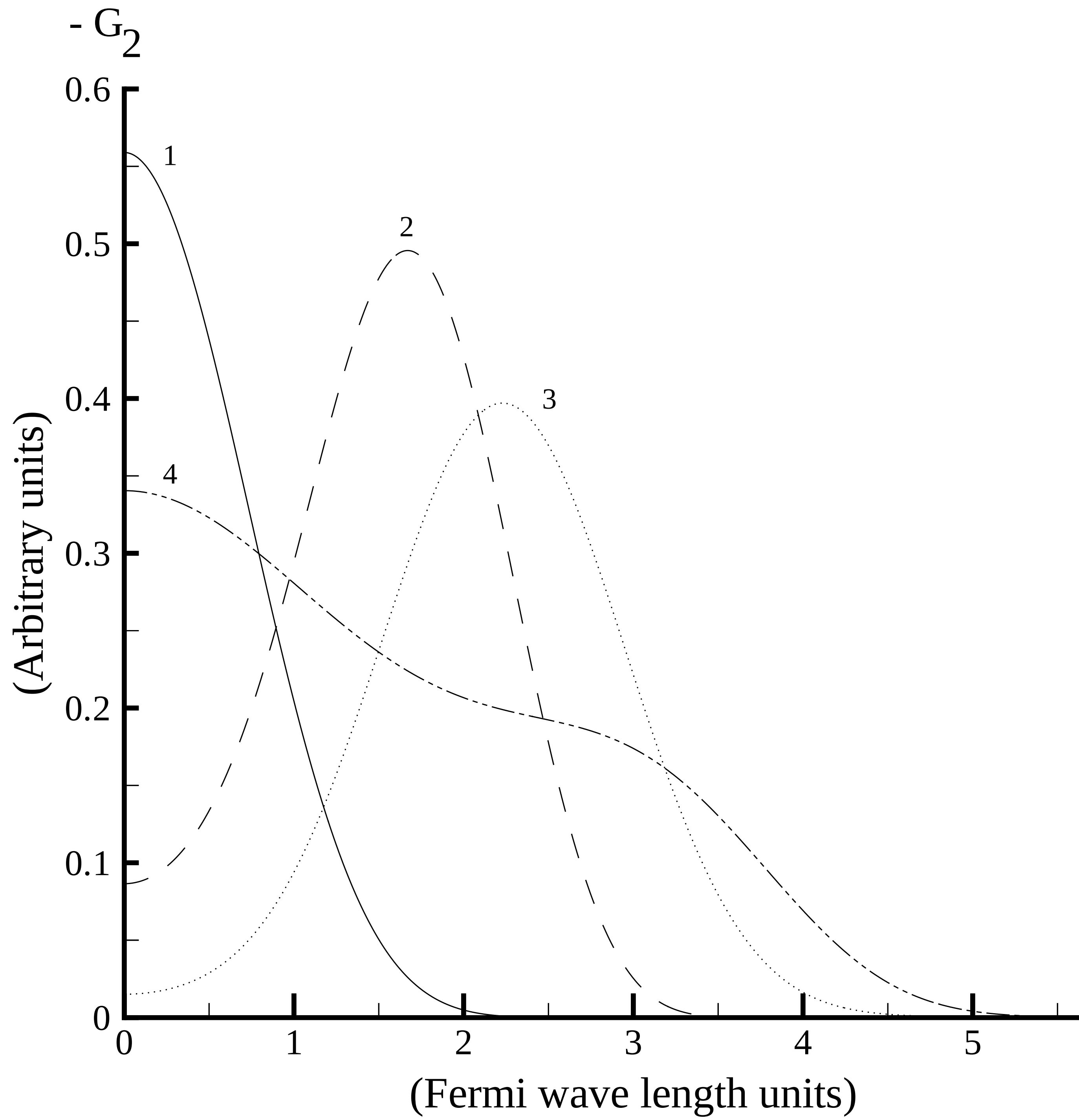
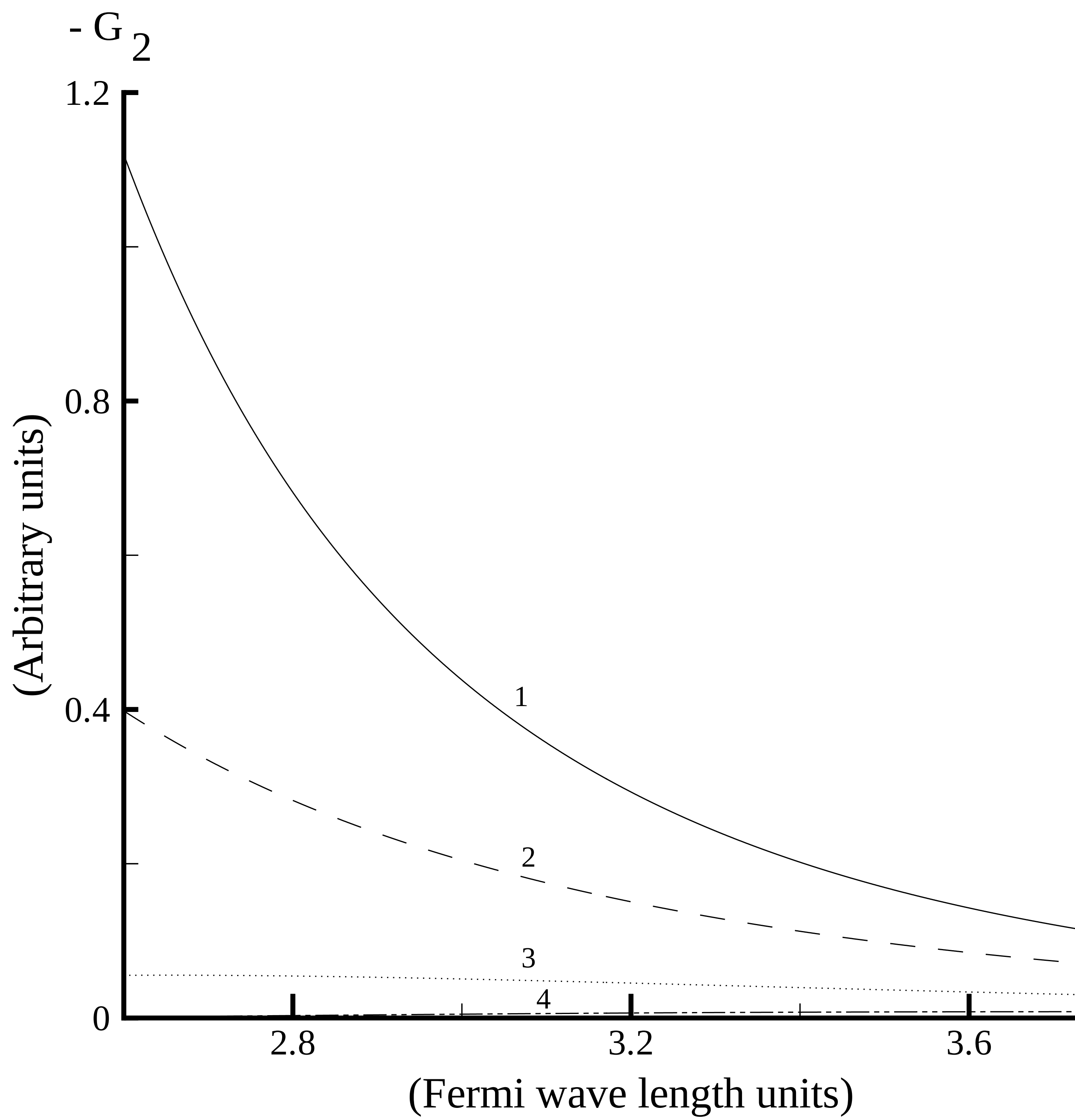


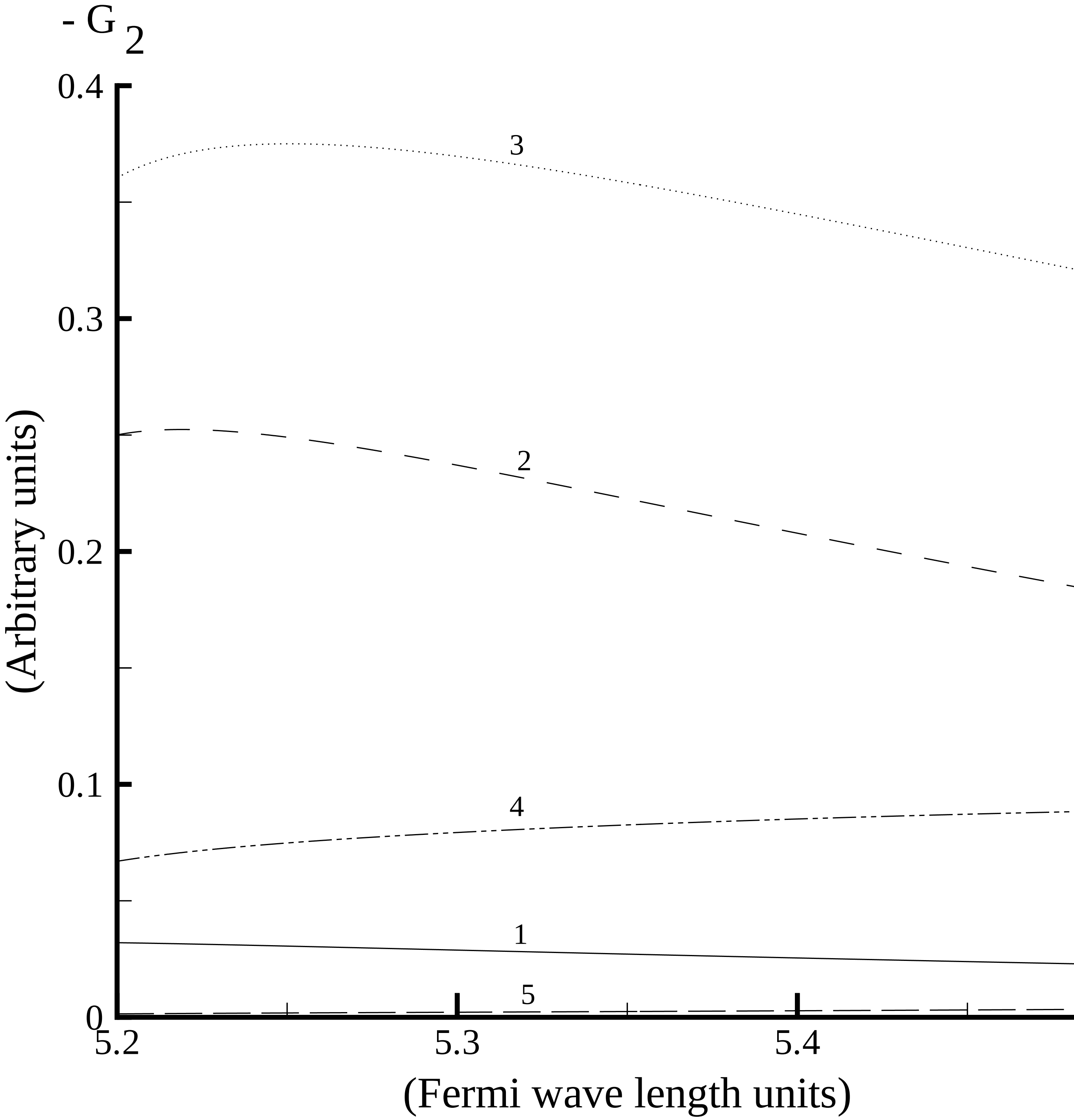
- G 2
(Arbitrary units)
1.2
0.8
0.4
0
0
0.005
0.01
0.015
0.02
1
2
3
4
(Fermi energy units)



- G2
(Arbitrary units)
0.6
0.5
0.4
0.3
0.2
0.1
0
1
2
3
4
0
1
2
3
4
5
(Fermi wave length units)



- G 2
1.2
0.8
0.4
0
(Arbitrary units)
1
2
3
4
2.8
3.2
3.6
(Fermi wave length units)



- G 2
(Arbitrary units)
0.4
0.3
0.2
0.1
0
3
2
4
1
5
5.2
5.3
5.4
(Fermi wave length units)